

Ethane, methoxy-d3
16995-14-5 | DTXSID20168777

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.60e-01

Global applicability domain: Inside

Local applicability domain index: 5.47e-01

Confidence level: 7.39e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propane, 1-methoxy-</div> <div>Measured: 1.21</div> <div>Predicted: 1.07</div>	<div>Image not found</div> <div>Ethylene glycol dimethyl ether</div> <div>Measured: -0.210</div> <div>Predicted: -0.109</div>	<div>Image not found</div> <div>Diethyl ether</div> <div>Measured: 0.89</div> <div>Predicted: 9.83e-01</div>
<div>Image not found</div> <div>1,4-Dioxane</div> <div>Measured: -0.270</div> <div>Predicted: -0.157</div>	<div>Image not found</div> <div>Dimethoxymethane</div> <div>Measured: 0.0</div> <div>Predicted: -0.0482</div>	